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       1578839 PROTEIN
       1085406 PROTEINS
       1828373 PROTEIN
                 (PROTEIN OR PROTEINS)
         23086 HYDROPHOBICITY
           784 HYDROPHOBICITIES
         23410 HYDROPHOBICITY
                 (HYDROPHOBICITY OR HYDROPHOBICITIES)
L1        6872 PROTEIN AND HYDROPHOBICITY

=> s l1 and (shift? (3a) hydrophobicity)
        402434 SHIFT?
         23086 HYDROPHOBICITY
           784 HYDROPHOBICITIES
         23410 HYDROPHOBICITY
                 (HYDROPHOBICITY OR HYDROPHOBICITIES)
            22 SHIFT? (3A) HYDROPHOBICITY
L2           8 L1 AND (SHIFT? (3A) HYDROPHOBICITY)

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L2   ANSWER 1 OF 8  CAPLUS  COPYRIGHT 2003 ACS on STN
AN   1995:561905  CAPLUS
DN   123:79182
TI   Glycosyl-phosphatidylinositol-anchored proteins exist in the
     plasma membrane of Chlorella saccharophila (Krueger) Nadson:
     plasma-membrane-bound nitrate reductase as an example
AU   Stoehr, Christine; Schuler, Frank; Tischner, Rudolf
```

CS Pflanzenphysiologisches Inst., Univ. Goettingen, Goettingen, D-37073, Germany
SO Planta (1995), 196(2), 284-7
CODEN: PLANAB; ISSN: 0032-0935
PB Springer
DT Journal
LA English
TI Glycosyl-phosphatidylinositol-anchored **proteins** exist in the plasma membrane of Chlorella saccharophila (Krueger) Nadson: plasma-membrane-bound nitrate reductase as an example
AB Expts. with plasma-membrane vesicles were performed in order to identify the attachment of hydrophobic nitrate reductase at the plasma membrane of C. saccharophila. The enzyme was successfully removed from the plasma membrane with phosphoinositol-specific phospholipase C, and showed cross-reactivity with a monoclonal antibody (clone aGPI-3) raised against the glycosyl-phosphatidylinositol (GPI) anchor of Trypanosoma variant surface **protein**. The enzyme was labeled in vivo by feeding [3H]ethanolamine to the cells and underwent an **hydrophobicity shift** after treatment with phosphoinositol-specific phospholipase C. The attachment of this form of nitrate reductase to the plasma membrane via a GPI anchor was demonstrated.
IT Cell membrane
Chlorella saccharophila
(glycosylphosphatidylinositol-anchored **proteins** exist in the plasma membrane of Chlorella saccharophila: plasma-membrane-bound nitrate reductase)
IT Glycophospholipids
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(phosphatidylinositol-contg., glycosylphosphatidylinositol-anchored **proteins** exist in the plasma membrane of Chlorella saccharophila: plasma-membrane-bound nitrate reductase)
IT 9013-03-0, Nitrate reductase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(glycosylphosphatidylinositol-anchored **proteins** exist in the plasma membrane of Chlorella saccharophila: plasma-membrane-bound nitrate reductase)

L2 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1993:560799 CAPLUS
DN 119:160799
TI Delineation of electrostatic- and hydrophobic-induced pKa shifts in polypentapeptides: the glutamic acid residue
AU Urry, D. W.; Peng, S.; Parker, T.
CS Lab. Mol. Biophys., Univ. Alabama, Birmingham, AL, 35294-0019, USA
SO Journal of the American Chemical Society (1993), 115(16), 7509-10
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB A common phenomenon in **protein** mechanisms is the occurrence of amino acid residues were shifted pKa values that are central to function in the particular **protein**. In order to understand **protein** mechanisms, it becomes essential to understand the dominant underlying mechanism whereby these large pKa shifts can occur. The most common explanation is based on the charge-charge repulsion mechanism, i.e., that the pKa shifts are electrostatic-induced. With this communication, a second mechanism for shifting pKa values is clearly delineated for the Glu residue; it is one of a hydrophobic-induced pKa shift arising from an apolar-polar repulsive free energy of hydration. Furthermore, the common exptl. diagnostic for the dominance of electrostatic interactions is found not to be so. In deducing the dominant forces, for example, that hold **protein** subunits together in a particular functional aggregate, a decrease in the assocn. const., on addn. of salt, has been diagnostic of the electrostatic

mechanism. The results, herein reported however, demonstrate in both the electrostatic and hydrophobic domains that addn. of salt can relax the pKa shifts. This indicates that the salt effect of decreasing assocn. can no longer be diagnostic of the electrostatic domain, but that a phenomenol. similar salt effect can also occur under conditions in which the hydrophobic domain is dominant.

IT **Hydrophobicity**
(pKa **shifts** in glutamic acid-contg. polypentapeptides induced by)

IT **Proteins**, properties
RL: PRP (Properties)
(pKa shifts in, electrostatic- and hydrophobic-induced pKa shifts in glutamic acid-contg. polypentapeptides as model for)

IT 7732-18-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrophobicity**, pKa **shifts** in glutamic acid-contg. polypentapeptides induced by)

L2 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1992:651752 CAPLUS
DN 117:251752
TI Design at nanometric dimensions to enhance **hydrophobicity** -induced pKa **shifts**
AU Urry, D. W.; Gowda, D. C.; Peng, S. Q.; Parker, T. M.; Harris, R. D.
CS Lab. Mol. Biophys., Univ. Alabama, Birmingham, AL, 35294-0019, USA
SO Journal of the American Chemical Society (1992), 114(22), 8716-17
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
TI Design at nanometric dimensions to enhance **hydrophobicity** -induced pKa **shifts**
AB Previously described has been a new mechanism of chemomech. transduction which results from a chem.-induced folding of **protein**-based polymers. Descriptively, the mechanism can be obsd. as the chem.-induced change in the temp. of an inverse temp. transition for hydrophobic folding and assembly. Mechanistically, it is considered to arise from the competition between apolar (hydrophobic) and polar (e.g., ionizable) residues for adequate hydration in structurally-constrained, water-limited matrixes such as **proteins**. The interaction energies on which the mechanism is based can be obsd. in terms of **hydrophobicity** -induced pKa **shifts**. The purpose of this communication is to report results on a set of **protein**-based polymers which were designed for the purpose of maximizing **hydrophobicity**-induced pKa **shifts**. The high mol. wt. polypentapeptides, actually polytricosapeptides in which six pentamers were either in fixed sequence or randomized, were designed to have the same amino acid compns. but with varied proximities between the one Glu residue and the five Phe residues per 30 residues. With only one Glu per 30 residues the charge-charge repulsion mechanism for pKa shifts is ruled out. Nonetheless, pKa shifts of up to 3.8 pH units were obsd. representing a free energy of interaction of 5 kcal/mol. To our knowledge, this is the largest pKa shift obsd. for a Glu residue, and it occurred when the five Phe residues were arranged around the Glu residue at 1 nm distances in the folded structure which contains some 50% water by wt. These results demonstrate the apolar-polar repulsive free energy of hydration to be of a sufficient magnitude to be a significant factor in **protein** structure and function.
ST **hydrophobicity** pKa **shift protein** based polytricosapeptide; polypeptide **protein** based **hydrophobicity** pKa **shift**; free energy interaction **protein** based polytricosapeptide
IT Free energy
(of interaction, of **protein**-based polytricosapeptides)
IT **Hydrophobicity**
(of **protein**-based polytricosapeptides)

IT Peptides, properties
RL: PRP (Properties)
(polytricosa-, **protein**-based, **hydrophobicity**-induced pKa **shifts** of)
IT **Proteins**, properties
RL: PRP (Properties)
(polytricosapeptides based on, **hydrophobicity**-induced pKa **shifts** of)
IT Protonation and Proton transfer reaction
(deprotonation, of **protein**-based polytricosapeptides, **hydrophobicity** in relation to)
IT 7732-18-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrophobicity**, of **protein**-based polytricosapeptides)
IT 125690-25-7 144227-24-7 144227-26-9 144227-28-1 144241-13-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrophobicity**-induced pKa **shifts** of)
IT 12408-02-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(protonation and Proton transfer reaction, deprotonation, of **protein**-based polytricosapeptides, **hydrophobicity** in relation to)

L2 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1992:485444 CAPLUS
DN 117:85444
TI **Hydrophobicity**-induced pK **shifts** in elastin **protein**-based polymers
AU Urry, Dan W.; Peng, Shao Qing; Parker, Timothy M.
CS Lab. Mol. Biophys., Univ. Alabama, Birmingham, AL, 35294, USA
SO Biopolymers (1992), 32(4), 373-9
CODEN: BIPMAA; ISSN: 0006-3525
DT Journal
LA English
TI **Hydrophobicity**-induced pK **shifts** in elastin **protein**-based polymers
AB Three polypentapeptides-poly[0.8(GVGVP), 0.2(GEGVP)], poly[0.8(GVGIP), 0.2(GEGIP)], and poly[0.75(GFGVP), 0.25(GEGVP)]-all analogs of the polypentapeptide of elastin-(Val1-Pro2-Gly3-Val4-Gly5)n or poly(VPGVG)-have been prepd. to det. the effect of changing the **hydrophobicity**, i.e., Val1 .fwdarw. Ile1 (I) and Val4 .fwdarw. Phe4 (F), on the pKa and the temp. dependence of pKa of the Glu(E) residue. Shifts on pKa as large as 1.7 units are obsd. and the temp. dependence is much steeper for the structure-dependent proximity of the more hydrophobic Ile1 residues to the Glu4 residue. Even though this system is dominated by the inverse temp. transition of hydrophobically driven folding on raising the temp., the effect of adding 0.15 N NaCl is to suppress the **hydrophobicity**-induced pKa **shift**.
ST elastin ionization **hydrophobicity** polypentapeptide model
IT Elastins
RL: PRP (Properties)
(ionization and temp. transition of, **hydrophobicity** effect on, polypentapeptides and modeling of)

L2 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1990:436136 CAPLUS
DN 113:36136
TI Involvement of denaturation-like changes in Pseudomonas exotoxin A **hydrophobicity** and membrane penetration determined by characterization of pH and thermal transitions. Roles of two distinct conformationally altered states
AU Jiang, Jean Xin; London, Erwin
CS Dep. Biochem. Cell Biol., State Univ. New York, Stony Brook, NY,

11794-5215, USA
SO Journal of Biological Chemistry (1990), 265(15), 8636-41
CODEN: JBCHA3; ISSN: 0021-9258
DT Journal
LA English
TI Involvement of denaturation-like changes in Pseudomonas exotoxin A **hydrophobicity** and membrane penetration determined by characterization of pH and thermal transitions. Roles of two distinct conformationally altered states
AB The effects of pH, temp., and denaturants were examd. to define the role of conformational changes in membrane penetration by the exotoxin. Two distinct low pH conformations exist. An intermediate low pH state (LI) dominates at pH 3.7-5.4 and is distinguished by blue-shifted fluorescence and weak or no **hydrophobicity**. The second low pH state (LII) is dominant below pH 3.7 and is characterized by red **shifted** fluorescence and strong **hydrophobicity**. LI is a folded state as judged by its spectroscopic properties and the observation that it undergoes distinct and cooperative thermal and denaturant-induced unfolding transitions. LII appears to be more like a denatured state, as it shows no cooperative thermal or denaturant-induced transitions and has spectroscopic properties very similar to exotoxin A that has been thermally denatured at pH 7. Exotoxin A in the LII state strongly binds detergent micelles and binds to and inserts into model membranes. Therefore, denaturation-like conformational changes appear to play an important role in membrane insertion. The pH of the transition to a membrane-inserting state is influenced by the compn. of the model membranes and is close to pH 5 in the presence of vesicles contg. a phosphatidylglycerol/phosphatidylcholine mixt. These vesicles probably promote formation of the LII state via mass action effects. The implications of these results for membrane penetration and translocation of **proteins** without apparent hydrophobic regions, such as exotoxin A, are discussed.
ST Pseudomonas exotoxin A **hydrophobicity** membrane penetration
IT Pseudomonas
(exotoxin A of, **hydrophobicity** in membrane penetrating activity of, denaturation-like changes in relation to)
IT Conformation and Conformers
(of Pseudomonas exotoxin, **hydrophobicity** and membrane penetrating activity in relation to)
IT Toxins
RL: BIOL (Biological study)
(exo-, A, of Pseudomonas, **hydrophobicity** and membrane penetrating activity of, denaturation-like changes in relation to)

L2 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1990:3497 CAPLUS
DN 112:3497
TI Mobility of secondary structure units of horse-muscle acylphosphatase. Relation to antigenicity
AU Saudek, Vladimir; Williams, Robert J. P.; Stefani, Massimo; Ramponi, Giampietro
CS Inorg. Chem. Lab., Univ. Oxford, Oxford, OX1 3QR, UK
SO European Journal of Biochemistry (1989), 185(1), 99-103
CODEN: EJBCAI; ISSN: 0014-2956
DT Journal
LA English
AB The antigenic properties of acylphosphatase were compared with its various sequential characteristics (**hydrophobicity**, chem. **shift** of the main-chain 1H NMR resonances, nos. and intensities of the nuclear Overhauser enhancements, H-D exchange, and sequential arrangement of the secondary structure units). The discussion is based on the complete sequential assignment of the 1H NMR spectrum and the knowledge of the 3-dimensional fold of the **protein** obtained by NMR spectroscopy from distance geometry calcns. Regions with very different degrees of

mobility could be distinguished. It was found that all major antigenic sites were located in the most mobile surface loops.

L2 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1985:484898 CAPLUS
DN 103:84898
TI Modulation of cell surface **hydrophobicity** in the benthic cyanobacterium Phormidium J-1
AU Bar-Or, Yeshaya; Kessel, Martin; Shilo, Moshe
CS Inst. Life Sci., Hebrew Univ. Jerusalem, Jerusalem, Israel
SO Archives of Microbiology (1985), 142(1), 21-7
CODEN: AMICCW; ISSN: 0302-8933
DT Journal
LA English
TI Modulation of cell surface **hydrophobicity** in the benthic cyanobacterium Phormidium J-1
AB A **shift** from cell-surface **hydrophobicity** to hydrophilicity was exptl. induced in the benthic hydrophobic cyanobacterium Phormidium J-1 by mech. shearing, chloramphenicol, and proteolytic treatment after preincubation with SDS. Treatment with SDS alone, while releasing large amts. of **protein** and carbohydrates from the cell wall, did not affect cell surface **hydrophobicity**. Ultrastructural anal. showed the cells to be enveloped by a double-layered minicapsule. Treatments affecting cell-surface **hydrophobicity** also caused changes in capsular components. A model, describing cell-surface structure, compn., and properties in Phormidium J-1, was constructed by correlating ultrastructural data with surface properties.
ST Phormidium surface **hydrophobicity** capsule; **protein** Phormidium surface **hydrophobicity**
IT Phormidium
(**hydrophobicity** of cell surface of)
IT Capsule, microbial
(**hydrophobicity** of Phormidium in relation to)
IT **Proteins**
RL: BIOL (Biological study)
(**hydrophobicity** of Phormidium in relation to, of cell surface)

L2 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1984:606733 CAPLUS
DN 101:206733
TI Membrane dopamine .beta.-hydroxylase: a precursor for the soluble enzyme in the bovine adrenal medulla
AU Helle, K. B.; Reed, R. K.; Pihl, K. E.; Serck-Hanssen, G.
CS Dep. Physiol., Univ. Bergen, Bergen, 5000, Norway
SO International Journal of Biochemistry (1984), 16(6), 641-50
CODEN: IJBOBV; ISSN: 0020-711X
DT Journal
LA English
AB Dopamine .beta.-hydroxylase (DPH) was monitored enzymically and immunol. in aq. and detergent-solubilized exts. of bovine adrenomedullary fractions. Degrdn. of the sol. DBH and acidic chromogranins by activation of endogenous proteases occurred during lysis in H2O. **Shifts** in the **hydrophobicity** of the membrane DBH were also apparent. Loss in enzyme **protein** or activity, on the other hand, was not obsd. for buffer-dialyzed chromaffin granules (pH 5-6). Limited proteolysis within the membrane phase, however, was indicated by the shift towards dominance of the intermediate hydrophobic DBH in the buffer-dialyzed chromaffin granules. By 2-dimensional, crossed immunoelectrophoresis with cationic detergent, the microsomal DBH was immunol. identical to the granule-bound enzyme but differed from the latter in mol. heterogeneity and in susceptibility to proteolytic solubilization by endogenous protease activities. DBH in the membranes of the chromaffin granules was proteolytically solubilized at pH 6-8 and the sol. DBH further degraded at

pH 5. Apparently, a post-translational conversion of the amphiphilic DBH into the sol. form, initiated at the level of the microsomes, may continue within the light and the heavy granule fractions which contain several DBH-converting and degrading proteolytic activities with acid optima.